

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188		
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1. REPORT DATE (DD-MM-YYYY) 18-12-2015		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 8-Dec-2014 - 7-Aug-2015	
4. TITLE AND SUBTITLE Final Report: 2014 Materials Research Society (MRS) Fall Meeting			5a. CONTRACT NUMBER W911NF-15-1-0022		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 611102		
6. AUTHORS Seung-Wuk Lee, Yongmin Liu, Robert Kaplar, Robert Lipton			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES Materials Research Society 506 Keystone Dr. Warrendale, PA 15086 -7573			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 66500-MS-CF.1		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT The world's foremost international scientific gathering for materials research, the MRS meeting showcased leading interdisciplinary research in both fundamental and applied areas, coordinated by over 200 scientists from both academia and industry in many countries around the world. The Meeting Chairs - Husam N. Alshareef (King Abdullah University of Science and Technology), Amit Goyal (Oak Ridge National Laboratory), Gerardo Morell (University of Puerto Rico), Jose A. Varela (University of Sao Paulo State - UNESP), and In Kyeong Yoo (Samsung Advanced Institute of Technology), put together a powerhouse program of 52 technical symposia in six					
15. SUBJECT TERMS Conference report, bio-inspired nanomaterials, Optical Metamaterials, Complex Oxides, Wide-Bandgap Materials, Computational materials science					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			J. Ardie Dillen
					19b. TELEPHONE NUMBER 724-779-2711

Report Title

Final Report: 2014 Materials Research Society (MRS) Fall Meeting

ABSTRACT

The world's foremost international scientific gathering for materials research, the MRS meeting showcased leading interdisciplinary research in both fundamental and applied areas, coordinated by over 200 scientists from both academia and industry in many countries around the world. The Meeting Chairs - Husam N. Alshareef (King Abdullah University of Science and Technology), Amit Goyal (Oak Ridge National Laboratory), Gerardo Morell (University of Puerto Rico), Jose A. Varela (University of Sao Paulo State - UNESP), and In Kyeong Yoo (Samsung Advanced Institute of Technology) - put together a powerhouse program of 52 technical symposia in six broad categories: Biomaterials and Soft Matter; Electronics and Photonics; Energy and Sustainability; Nanomaterials and Synthesis; Theory, Characterization, and Modeling; and General Materials and Methods. Highlights included: Tutorial T, Always dedicated to the materials community, Hiroshi Amano of Nagoya University served as an instructor on nitride-based LEDs before traveling to Stockholm for the Nobel Prize ceremony; Materials Hackathon: For the first time, MRS held a 24-hour competition to create software to solve materials-related challenges; Innovation and Inclusion: What It Takes to Move Diversity Forward, Vern Myers, Esq., principal of Vern Myers Consulting Group, LLC, engaged participants in an interactive session about culturally effective habits that will help promote diversity in scientific organizations. Organized by the Women in Materials Science & Engineering Subcommittee, this session was open to women and men.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 680.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

NONE

Graduate Students

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Names of Under Graduate students supported

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

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Technology Transfer

Interactions with invited speakers from national laboratories, DOE.

Final Report to the Army Research OfficeBlock Grant Funding

Symposium F: Reverse Engineering of Bio-Inspired Nanomaterials
Grant Number: W911NF-15-1-0022

Prepared by: Dr. Seung-Wuk Lee,
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University of California, Berkeley
220 Donner Laboratory
Berkeley, CA 94720
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On behalf of all Symposium R Organizers:

Lara Estroff, Cornell University
Seung-Wuk Lee, University of California, Berkeley
Jwa-Min Nam, Seoul National University
Edward Perkins, U. S. Army Corps of Engineers

1. Background:

Nature has been a source of great inspiration for many scientists and engineers to solve challenging scientific and engineering problems. The field of bioinspired materials has made great progress over the last decade. This field focuses on pursuing a fundamental understanding of the materials design principles in nature using basic biological building blocks (i.e, DNA/RNA, peptide/proteins, lipids, and sugars) and re-engineering hierarchically organized functional structures for various applications. Progress in bio-inspired or biomimetic materials design provides new solutions to tackle challenging scientific problems in energy, medicine, nanomanufacturing, sensors and novel hard materials. Furthermore, reverse engineering of the lessons from nature creates many novel functional applications including DNA-origami, programmable peptide/protein engineering, design of organic/inorganic hybrid composite materials, and novel hybrid nanomaterials for sensor, actuators, diagnostics, and therapeutics.

2. Symposium goals:

The primary goal of this symposium proposal was to seek travel support for graduate students, post-docs, young faculty, and invited speakers to attend the symposium on “Reverse Engineering of Bio-Inspired Nanomaterials” at the Fall MRS meeting in Boston, MA, November 30-December 5, 2014.

3. Symposium Attendance:

We had a 3-day symposium (Dec. 1st-3rd) during the Material Research Society Meeting. The symposium was composed of 19 invited talks and 35 oral presentation and 47 posters. The symposium offered opportunities for investigators to present their research and engage with others on an individual and informal basis. To assure the highest quality presentations, submitted papers were carefully critiqued and accepted (Among 120 papers, we accepted 101 papers and 19 were rejected).

4. Symposium Highlight:

We are very happy to report that a diverse set of research was presented in the symposium, covering a wide range of research at the forefront of bio-inspired nanomaterials. In particular, we highlighted that the history of the bionanomaterials in DNA, peptide/proteins, lipids, and cells and their applications in various biomedical, biosensing, and bioenergy applications. We believe that this turned out to be a successful approach that was highly beneficial for the goals of Symposium F.

Here are of highlights of the talks:

Joanna Aizenberg (Harvard Univ.) discussed bio-inspiration for the design of responsive functional nanomaterials to control material properties; **Angela Belcher** (Massachusetts Inst. of Technology) discussed the exploitation of directed evolution of bacteriophage to synthesize radically novel electronic and battery devices at protein and semiconductor interfaces. **Ashutosh Chilkoti** (Duke Univ.) discussed rational design of protein-based matrices for the control of their physico-chemical properties and their spatial and temporal organization at molecular dimensions. **Timothy Deming** (Univ. of California-Los Angeles) discussed chemical synthesis of monodisperse multi-block copolypeptides for the well-defined hierarchical structure and medical and nanostructured materials. **Trevor Douglas** (Montana State Univ.) discussed the synthesis of nanoparticles and their self-assembly on the protein cage of various virus-based materials for medical and electronic application. **Oleg Gang** (Brookhaven National Lab) discussed the novel way to design super lattice structure fabrication from the sequence specific DNA oligomer and gold nanoparticles to create the DNA-assisted molecular structures and their crystallization growth mechanism. **Sarah Heilshorn** (Stanford Univ) discussed the synthesis and characterization of protein- and peptide-based materials guide and direct cellular morphology for the tissue engineering and regenerative medicines. **David Kaplan** (Tufts Univ.) discussed the understanding and controlling of the biological synthesis and processing of biopolymers and biopolymer interfaces, which can be used to control the functional attributes of the polymers related to cell responses, solution properties, and architectural control of assembly. **Phillip Messersmith** (Northwestern University) discussed bioadhesive material design inspired from the mussel proteins and their reverse engineering for the tissue engineering and super glue materials. **Francesco Stellacci** (EPFL, Switzerland) discussed synthesis and characterization of the lipid stripe engineered nanoparticles for the drug delivery and catalyst development. **Nadrian Seeman** (NYU) discussed the DNA-based nanostructures development and characterization for the DNA-based machines, switches, walkers, and computing. **Samuel Stupp** (Northwestern Univ.) discussed supramolecular self-assembly of peptide amphiphiles to activate cells for differentiation into the phenotypes of mineralized tissues such as bone, dentin, and enamel.

Among the student presentation, we selected four best presentations for graduates and postdocs. The best presentation recipients were Yuanyuan Zhao (City Univ. of New York), Minkyu Kim (MIT), and Vivek Kumar (Seoul National Univ., Malav Desai (UC Berkeley).

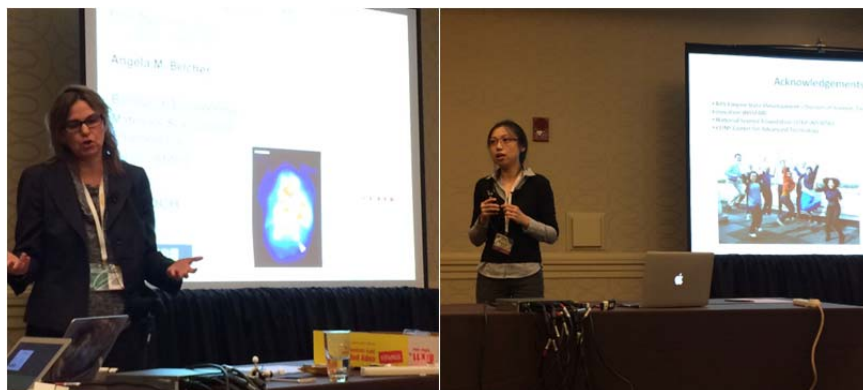


Figure: (Left) Dr. Angela Belcher discussed the virus-based energy producing materials. (Right) Ms. Yuanyuan Zhao discussed about he bio-inspired stimuli-responsive polymeric materials.

5. Funding Allocation

We raised a total of \$9,500 funding support from ARO (\$4,000), NSF (\$4,000) and MRS (1,500). Funding from the ARO was allocated to support 10 travel grants for the invited speaker (\$400). Funding from NSF and MRS supplemented travel grants and student best presentations.

6. Future perspective:

The symposium provided a forum for scientist and engineers who use biological building blocks or bio-inspiration as a critical component in current and emerging technologies ranging from drug delivery, and tissue engineering, to molecular electronics and nanotechnology. In addition, this symposium promoted cross-fertilization of ideas and technologies encompassing different disciplines including chemistry, physics, biology, materials science, electric engineering. It also focused on new innovative biological tools and the biomolecular materials discipline that applied principles of biomaterials or their self-assembled structures to the development of technologically useful materials. Most importantly, the symposium facilitated opportunities for junior faculties, postdoctoral fellows, graduate students and researchers from underrepresented groups to present research results in an interdisciplinary and dynamic national symposium. We believe that bio-inspiration is a great tool to provide a various of solution for the future challenges in energy, security, and health related issues. We need to foster the fundamental research efforts and their tangible applications to sustain the further research in bionanoscience and bionanotechnology in the future.

Further details on the symposium program may be found at:

<http://www.mrs.org/fall-2014-program-f/>

e-Proceedings for Symposium F may be viewed here:

<http://journals.cambridge.org/action/displayIssue?jid=OPL&volumeId=1722&iid=9696784>

MRS ONLINE PROCEEDINGS LIBRARY - 2015 - VOLUME 1722

MgO Nanomaterials Improve Fibroblast Adhesion and Proliferation
Daniel J. Hickey and Thomas J. Webster

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f05-13](#)

doi: 10.1557/opl.2015.438, Published online by Cambridge University Press 11 May 2015

Computational modeling of bacteriophage self-assembly during formation of hierarchical structures

Christopher M Warner and Olexandr Isayev and Aimee R. Poda and Michael F. Cuddy and Wayne D Hodo and Seung-Wuk Lee and Edward J Perkins

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f05-28](#)

doi: 10.1557/opl.2015.428, Published online by Cambridge University Press 12 May 2015

Bio-hybrid photoconverter by covalent functionalization of the photosynthetic reaction center of *Rhodobacter sphaeroides* with fluorescein isothiocyanate

Rocco Roberto Tangorra and Alessandra Antonucci and Francesco Milano and Simona la Gatta and Alessandra Operamolla and Roberta Ragni and

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f05-51](#)

doi: 10.1557/opl.2015.602, Published online by Cambridge University Press 16 Jun 2015

The Gating Mechanism of Mechanosensitive Channels in Droplet Interface Bilayers

Joseph S. Najem and Eric Freeman and Sergei Sukharev and Donald J. Leo

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f05-49](#)

doi: 10.1557/opl.2015.601, Published online by Cambridge University Press 16 Jun 2015

M13 Bacteriophage Biolaminates for Nanomaterials with Improved Stiffness

Christopher M. Warner and Amitabh Ghoshal and Michael F. Cuddy and Aimee R. Poda and Natalie D. Barker and Daniel E. Morse and Seung-Wuk Lee and Edward J. Perkins

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f11-03](#)

doi: 10.1557/opl.2015.603, Published online by Cambridge University Press 16 Jun 2015

Model Neural Membrane Droplet Interface Bilayers from Brain Total Lipid Extract for Studying Membrane-Peptide Interactions with Amyloid- β

Graham J. Taylor and Stephen A. Sarles

[MRS Online Proceedings Library, Volume 1722, 2015, mrsf14-1722-f08-03](#)

doi: 10.1557/opl.2015.429, Published online by Cambridge University Press 12 May 2015



Final Technical Report to the Army Research Office

Grant Number: W911NF-15-1-0022

Symposium L (Optical Metamaterials and Novel Optical Phenomena Based on Nanofabricated Structures)
MRS 2014 Fall Conference

Organizers: Yongmin Liu (Northeastern University), Federico Capasso (Harvard University), Andrea Alù (The University of Texas at Austin), Mario Agio (National Institute of Optics)

Optical metamaterials have witnessed a significant progress in the past decades. Their unique properties provide a wide range of physical, optical, and electronic phenomena to explore for scientists and engineers, including negative refraction, sub-diffraction-limited imaging, invisibility cloaking, strong chirality, and optical nonlinearity management. Consequently, optical metamaterials promise novel applications in optics and photonics, which embraces light emission and propagation, modulation and detection, sensing, imaging, energy harvesting, photocatalysis, and more recently the exploration of quantum phenomena.

The objectives of this symposium were to bring together researchers from different disciplines, including physics, materials science, engineering, chemistry and biology, to share recent breakthroughs, identify critical issues, and exchange ideas for future directions in the field of optical nanostructured metamaterials and plasmonics. We had structured the program to attract contributions on fundamental theory and new concepts, emerging nanofabrication techniques and architectures, novel devices, and applications.

The symposium was extremely successful. We received about **200** abstract submissions, and finally ended up with a five-day technical program. In total, we had **18** invited talks, about **80** contributed talks and **80** poster presentations with almost **200** participants, making our symposium among the largest ones in recent MRS conferences on similar topics. Seven manuscripts were published in MRS proceeding. In addition, we successfully organized a full-day tutorial on *Metamaterials and Plasmonics: from Fundamentals to Applications* given by four distinguished lecturers in the field (Prof. David R. Smith at Duke University, Prof. Shuang Zhang at University of Birmingham, Prof. Harry Atwater at Caltech, and Prof. David A. B. Miller at Stanford University). The tutorial attracted a number of colleagues and students who are interested in this field while at different levels. Further details on the symposium programs can be found at <http://www.mrs.org/fall-2014-program-l/>

The symposium presentations represented the frontier research in the field. For instance, our symposium featured work on nanophotonics and plasmonics based on emerging 2D materials; new research on meta-molecules and 3D metamaterial design for reconfigurable or adaptive materials; planar optics based on 2D optical metamaterials, so-called metasurfaces, for both near-field and far-field wave engineering; new work on plasmonics-enabled quantum nano-optical control and ultrasensitive detection; and emerging synthesis and fabrication techniques for

scalable production of multifunctional metamaterials. Much of the work presented is either sponsored or closely related to the mission of ARO. For example, the Optics and Fields Program of the Physics Division targets remote sensing, information processing, light and energy transmission, as well as new and emerging phenomena based on optical metamaterials. The Optoelectronics Programs of the Electronics Division focuses on high-data-rate optical networks, optical interconnects, new lasers, efficient and high-speed switching, emitters and architectures for novel display and imaging based on optical nano-architectures.

Our symposium served as a broadest forum worldwide to summarize the most recent breakthroughs in optical metamaterials and plasmonics, and to address the most prominent challenges in these fields. Furthermore, considering the wide scope of metamaterial and plasmonics research, our symposium also provided an inspiring environment to facilitate the interaction between scientists and engineers across different disciplines in the materials society as well as industry. For instance, from the symposium we have seen rapid development and great potential in photonics and plasmonics based on 2D materials. We are also excited about the plasmonics-mediated carrier dynamics at the single molecular level, and its implication in chemical energy harvesting. These directions are certainly worth of further exploration.

We highly appreciate the financial support from ARO for our symposium. The grant was used to support three outstanding graduate students, eight invited speakers, and four tutorial instructors. We particularly encouraged and facilitated the participation of students and young scientists.

Portions of Symposium L were video-recorded and may be viewed here:

<http://www.prolibraries.com/mrs/?select=sessionlist&conferenceID=12&packageID=111>

e-Proceedings for Symposium L may be viewed here:

<http://journals.cambridge.org/action/displayIssue?jid=OPL&volumeId=1728&iid=9542722>

MRS ONLINE PROCEEDINGS LIBRARY - 2015 - VOLUME 1728

Photonic coupled systems between on-chip integrated microresonator and core-shell nanoparticle
Y. Xiong and P. Pignalosa and Y. Yi

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I03-16](#)

doi: 10.1557/opl.2015.14, Published online by Cambridge University Press 30 Jan 2015

Degradation in aluminum resonant optical rod antennas

Patrick M. Schwab and Carola Moosmann and Katja Dopf and Konstantin S. Ilin and Michael Siegel and Uli Lemmer and Hans-Juergen Eisler

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I15-04](#)

doi: 10.1557/opl.2015.40, Published online by Cambridge University Press 05 Feb 2015

Coupling of single DBT molecules to a graphene monolayer: proof of principle for a graphene nanoruler

G. Mazzamuto and A. Tabani and S. Pazzagli and S. Rizvi and A. Reserbat-Plantey and K. Schädler and G. Navickaite and L. Gaudreau and F.S. Cataliotti and F. Koppens and C. Toninelli

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I06-02](#)

doi: 10.1557/opl.2015.169, Published online by Cambridge University Press 23 Feb 2015

Guided-mode resonance and field enhancement in semiconductor nanorod arrays

W. X. Yu and Y. Yi

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I03-17](#)

doi: 10.1557/opl.2015.358, Published online by Cambridge University Press 21 Apr 2015

Implementation of CVD Diamond Growth Methods for Selective and Efficient Formation of Color-Centers in Diamond

Stefano Gay and Giacomo Reina and Ilaria Cianchetta and Emanuela Tamburri and Mariglen Angjellari and Maria Letizia Terranova and Silvia Orlanducci

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I12-07](#)

doi: 10.1557/opl.2015.262, Published online by Cambridge University Press 16 Mar 2015

Enhanced selective thermal emission with a meta-mirror following Generalized Snell's Law

M. Ryyan Khan and Xufeng Wang and Enas Sakr and Muhammad A. Alam and Peter Bermel

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I02-09](#)

doi: 10.1557/opl.2015.357, Published online by Cambridge University Press 21 Apr 2015

Fabrication of Rough Polymer Surfaces Exhibiting Anti-reflective Properties

Srinadh Mattaparthi and Chandra S. Sharma

[MRS Online Proceedings Library, Volume 1728, 2015, mrsf14-1728-I14-13](#)

doi: 10.1557/opl.2015.190, Published online by Cambridge University Press 27 Feb 2015



Symposium N, Frontiers in Complex Oxides, focused on emergent and future developments in the broad field of complex oxides materials and their applications with the intent of bringing together scientists from different disciplines – theorists and experimentalists – and encouraging discussions at the cross-disciplinary level. Complex oxides have fascinated researchers for decades because their highly tunable structures and properties can be engineered for many different applications, from low-power electronics to efficient energy conversion devices. Recent advances in theory, synthesis and characterization are unlocking surprising new phenomena (magnetism or metallicity at interfaces between non-magnetic/insulating oxides, for example) and revealing new possibilities for applications. The goal of this symposium was not only to highlight current state of the art advances, but also to stimulate discussions on future directions. Oral and poster presentations were given by academics, members of industry, as well as Department of Energy Laboratories with varied expertise and experience, i.e. junior faculty, postdocs, and graduate students.

Two of the highlighted talks follow:

Coupling of Epitaxial Strain and Oxygen Content in Multifunctional Oxide Thin Films
Tricia Meyer, Oak Ridge National Laboratory

Tricia Meyer shared the discoveries that her team at Oak Ridge National Laboratory (ORNL) recently made concerning lanthanum strontium copper oxide materials and the key factors that govern their superconductive behaviors. In particular, the property is a nexus of three key factors: lattice parameter, oxygen content, and mechanical strain on the superconductivity. Transport measurements confirmed a significant modulation of carrier concentrations especially by tensile strain in these complex oxides. Meyer manipulated the concentrations of oxygen vacancies using vacuum and oxygen annealing and found a strong correlation between the oxygen voids in the lattice and carrier densities. A theoretical density functional theory approach highlighted different activation barriers, which diverge depending on the type of strain, correlated with electronic structures of these materials. By combining experimental and theoretical efforts, the ORNL team discovered that applying tensile strain to the cuprates significantly reduces the oxygen vacancy formation energy, subsequently depleting hole carriers due to preferential loss of oxygen at a particular sub-lattice site (equatorial): whereas compressive strain increased the oxygen activation energy barrier, robustly maintaining the oxygen stoichiometry. Meyer suggested that the strong coupling among strain, oxygen stoichiometry, and lattice distortion is primarily responsible for the presence or absence of superconductivity. These findings provide novel insights into complex perovskites and unique properties that more members of this materials family may possess.

Direct Characterization of Ferroelastic Domain Motion in Bismuth Ferrite under Varying Epitaxial Strain States

Michael Jablonski, Drexel University

Ferroelectric materials find use in a number of advanced electronic applications such as ferroelectric random-access memory, sensors, and capacitors. While these materials have been investigated for nearly a century, the mechanisms governing the unique effects in ferroelectric systems are not yet fully understood. Toward this end, Michael Jablonski and colleagues have investigated thin films of bismuth ferrite layered by molecular beam epitaxy. Using high-resolution transmission electron microscopy (TEM) imaging, they were able to capture the dynamic domain wall movement at extremely fast timescales. Domain nucleation was seen to occur at misfit dislocations and growth occurred first along its axis. The researchers saw that applying a positive or negative bias, favorably switched domain walls of certain orientations. TEM imaging coupled with geometric phase analysis identified enhanced strain concentrations at domain wall intersections that may lead to strong domain pinning. This work provides further insight into the operation of ferroelectric materials through unique *in situ* biasing experiments.

MRS ONLINE PROCEEDINGS LIBRARY - 2015 - VOLUME 1730

The Direct Measurement of Ionic Piezoresistance

Stuart N. Cook and Harry L. Tuller

[MRS Online Proceedings Library, Volume 1730, 2015, mrsf14-1730-n10-05](#)

doi: 10.1557/opl.2015.266, Published online by Cambridge University Press 16 Mar 2015

Simultaneous Spectroscopic, Diffraction and Microscopic Study of the Metal-Insulator Transition of VO_2

J. Laverock and S. Kittiwatanakul and A. A. Zakharov and Y. R. Niu and B. Chen and J. Kuyyalil and S. A. Wolf and J. W. Lu and K. E. Smith

[MRS Online Proceedings Library, Volume 1730, 2015, mrsf14-1730-n05-04](#)

doi: 10.1557/opl.2015.480, Published online by Cambridge University Press 21 May 2015

Oxygen Vacancies at the $\gamma\text{-Al}_2\text{O}_3/\text{STO}$ Heterointerface Grown by Atomic Layer Deposition

Thong Q. Ngo and Martin D. McDaniel and Agham Posadas and Alexander A. Demkov and John G. Ekerdt

[MRS Online Proceedings Library, Volume 1730, 2015, mrsf14-1730-n08-06](#)

doi: 10.1557/opl.2015.294, Published online by Cambridge University Press 19 Mar 2015

Evolution of correlated electron behavior from the surface to the bulk in $\text{Sr}_x\text{Ca}_{1-x}\text{VO}_3$

J. Laverock and B. Chen and J. Kuyyalil and R. P. Singh and G. Balakrishnan and R. M. Qiao and W. L. Yang and J. Adell and B. Karlin and J. C. Woicik and K. E. Smith

[MRS Online Proceedings Library, Volume 1730, 2015, mrsf14-1730-n06-08](#)

doi: 10.1557/opl.2015.265, Published online by Cambridge University Press 16 Mar 2015



Report to Army Research Office (ARO)

MRS 2014 Fall Meeting, Boston, MA, November 30 – December 5, 2014

Symposium T: Wide-Bandgap Materials for Solid-State Lighting and Power Electronics

Robert Kaplar (Sandia National Labs; lead organizer and author of this report)

Burak Ozpineci (Oak Ridge National Lab)

Gaudenzio Meneghesso (University of Padova)

Tetsuya Takeuchi (Meijo University)

Overview

Symposium T consisted of tutorial, oral, and poster presentations covering topics in wide-bandgap materials targeted at solid-state lighting and power electronics applications. The call papers is posted on the MRS web site at <http://www.mrs.org/fall-2014-call-for-papers-t/>. The majority of the technical sessions focused on the III-N materials family, although half of one day was devoted to SiC for power electronics; one-third of the tutorial day covered this topic, as well. Additionally, one session covered “novel” WBG materials such as Ga₂O₃. Further, half of one day was devoted to a joint session with Symposium AA, “Synthesis, Processing, and Mechanical Properties of Functional Hexagonal Materials for Energy Applications”. Finally, 17 papers from the symposium were published electronically as MRS Proceedings Volume 1736 (available at <http://journals.cambridge.org/action/displayIssue?jid=OPL&volumeId=1736&iid=9479921>).

Relevance to ARO

The research presented in this symposium was relevant to several of ARO’s interests within the sensors and electron devices organization. The symposium was designed to be well-aligned with ARO’s long-standing interest in forefront electronic materials and devices. For optoelectronics, applications of WBG materials include advanced electro-optical technologies (including both emitters and detectors) and flexible displays. For power electronics, higher voltage and current capability in a smaller volume (improved size, weight, and power, i.e. better SWaP) compared to what can be achieved with Si-based power electronics is a key advantage that will be enabled by WBG materials, resulting in improvements in electric vehicles, pulsed power, directed energy, and portable power for soldiers and forward operating bases.

Use of ARO Funds

The ARO funds were used to provide travel and registration support to the tutorial and invited speakers. This support was crucial, as a few of the speakers indicated that they would have had difficulty justifying their attendance at the meeting had this funding not been available. The tutorial and invited speakers formed the backbone of a successful and high-quality symposium, and as such the symposium is very grateful for the funding. The assistance of the MRS staff in facilitating the funding is likewise gratefully acknowledged.

Tutorial Program

The tutorial program comprised the entire day on Sunday, November 30 and featured three sections, each two hours in duration:

1. SiC for Power Electronics (Dr. Victor Veliadis, Northrop-Grumman Electronic Systems)
2. GaN-Based Power Devices: Trapping, Breakdown, and Reliability Issues (Prof. Matteo Meneghini, University of Padova)
3. Fundamental Physics of Nitride-Based Optoelectronic Devices (Prof. Hiroshi Amano, Nagoya University)

The tutorial program was designed to cover the two primary materials of interest (SiC and the III-N family) as well as the two main applications areas for these materials (as indicated in the title of the symposium). The tutorials were well-attended. Notably, Prof. Amano's talk was quite popular, due to his having won the 2014 Nobel Prize in Physics a few months prior to the meeting. The tutorial slides, which were made available to attendees, are a fairly comprehensive resource, and since the meeting I have found myself referring to them often in the course of my own work.

Technical Program

The technical program consisted of 12 oral sessions as well as a poster session. Highlights of each session are described below. Note that the full program (including the abstracts) is available at <http://www.mrs.org/fall-2014-program-t/>.

Session 1: GaN Power Devices 1

This session featured three invited talks: Martin Kuball (University of Bristol, UK) covering defects and reliability in GaN HEMTs; Oleg Laboutin (IQE) covering GaN growth on Si substrates; and Tomas Palacios (MIT) covering design, fabrication, and testing of GaN transistors and diodes. Six contributed talks rounded out the session, with notable contributions from Georgia Tech on thermal resistance of interfacial layers in GaN epilayers on Si, and Ohio State and Vanderbilt on proton irradiation of GaN HEMTs.

Session 2: GaN Power Devices 2

This session was a continuation of Session 1 and featured four invited talks: David Brown (HRL Labs) covering design and processing of AlGaIn and GaN HEMTs for power and RF applications; Steve Kaun (UC Santa Barbara) covering growth of (Al,In,Ga)N alloys and heterostructures for power devices by plasma-assisted MBE; Russ Dupuis (Georgia Tech) covering bipolar GaN power devices; and Isik Kizilyalli (Avogy) covering vertical GaN power devices grown on GaN substrates. Three contributed talks completed the session.

Session 3: UV Optoelectronics

This session featured a single invited talk by Andy Allerman (Sandia) covering the MOCVD growth and processing of low-dislocation-density AlGaIn templates for UV laser diodes. The session also featured six contributed talks; of note were a talk from NC State University and the Army Research Office on high reflectivity AlN/AlGaIn DBRs for vertical UV lasers, and a talk from the Universities of Paderborn and Magdeburg (Germany) on cubic GaN/AlN MQWs.

Session 4: LEDs for Solid-State Lighting 1

This session featured three invited talks: Shunsuke Ishizawa (Sophia University, Japan) on InGaIn-based nano-column emitters; Matteo Meneghini (University of Padova, Italy) on radiative and non-radiative loss mechanisms in InGaIn-based LEDs, and Yasufumi Fujiwara (Osaka University, Japan) on red light emission in Eu-doped GaIn. Six contributed talks completed the session, including one from Northwestern University and Sandia on nano-structural analysis of InGaIn QWs.

Session 5: Poster Session

The poster session featured 14 posters covering a wide variety of topics relevant to the symposium. Highlights include a poster from the University of Idaho and Washington State University on the use of ZnO for optoelectronics, and a poster from the Korea Research Institute of Standards and Science and Chungnam National University (also in Korea) on the use of x-ray transmission topography to assess the degree of surface damage in sapphire substrate wafers.

Session 6: SiC Power Devices

This session featured four invited talks: Anant Agarwal (Department of Energy) covering manufacturing of WBG power devices; Aivars Lelis (Army Research Lab) covering SiC MOSFET reliability; Pat Lenahan (Penn State) covering point defects at and near the SiC-SiO₂ interface; and Sarit Dhar (Auburn) covering channel transport physics in SiC MOSFETs. Three contributed talks completed the session; of note was an interesting talk from Carnegie Mellon and the University of South Carolina on the glide of threading edge dislocations in 4H-SiC during epitaxial growth.

Session 7: LEDs for Solid-State Lighting 2

An invited talk in this already short session had to be cancelled, leaving only two contributed talks. One of these, from Korean University and the University of Florida, highlighted GaIn LEDs grown on flexible substrates. The second of these, from Rutgers

University, the Chinese Academy of Sciences, Jiangsu University, and Lawrence Berkeley National Lab described work on a new rare-earth-free yellow phosphor for white LEDs.

Session 8: Novel WBG Materials

This session featured three contributed talks on materials other than SiC and the III-N family that have potential applicability to lighting and/or power electronics. The first of these, from the Tokyo Institute of Technology as well as the Toshima and Roca companies and the Kanagawa Industrial Technology Center (all in Japan) described the growth of Ga₂O₃ by pulsed UV laser annealing. The second, from Osaka University (Japan), described the use of ZnSe, ZnO, and CdSe microspheres for lasing; and the third, from MIT, described the use of 2.1 eV AlInP for optoelectronics.

Session 9: T/AA Joint Session 1, Optical Properties of III-N Materials

The first of two joint sessions with Symposium AA, this session featured two invited talks: Shigefusa Chichibu (Tohoku University, Japan in collaboration with NC State and Hexatech) covering spatial-time-resolved cathodoluminescence of AlN epitaxial films; and Liverios Lymperakis (Max Planck Institute in collaboration with the Leibniz Institute for Crystallography, Germany) on excitonic emission from screw dislocations in GaN. The session concluded with two contributed talks, including one from NC State and Hexatech on photo-pumped UV-C lasers grown on AlN substrates.

Session 10: T/AA Joint Session 2, Semi-Polar and Bulk Growth of III-Nitrides

The second of the two joint sessions with Symposium AA, this session had a single invited talk (Ferdinand Scholz, University of Ulm, Germany) on the growth of semi-polar GaN heterostructures on patterned sapphire substrates. The session concluded with three contributed talks, including one from Georgia Tech and Arizona State on stimulated emission in AlGa_N lasers grown on sapphire substrates, and another growth, doping, and characterization of bulk AlN crystals from the Leibniz Institute for Crystal Growth in Berlin, Germany.

Session 11: Non-Polar III-N Structures

This session had four contributed talks. Of note was a talk from Penn State on a method for fabricating non-polar GaN on (001) Si using etched trench arrays. Also significant was a talk from Seoul University (Korea) and the Naval research Lab on the chemical etching behavior of polar, semi-polar, and non-polar GaN films.

Session 12: III-N Defect and Transport Physics

This session featured a single invited talk (Andy Armstrong, Sandia) on deep-level defects in III-N materials. The session also had four contributed talks, including by Doug Irving (NC State, in collaboration with Hexatech, the Tokyo University of Agriculture and Technology,

and Tokuyama Corporation) on point the properties of point defects and point defect complexes in AlN and AlGaN as predicted by density-functional theory.

Session 13: III-N Epitaxy

An invited talk by Nobel Prize winner Prof. Hiroshi Amano (who had given the tutorial several days prior) unfortunately had to be cancelled; this is because Prof Amano had to leave the MRS meeting early to prepare for the Nobel Prize ceremony in Sweden! This left the session with seven contributed talks. Notable among these was a talk by Nazmul Arefin of Oklahoma State University on growth of GaN on sapphire, (111) Si, and (111) SiGe using a pulsed electron beam deposition process. Also significant was a talk by Zakaria Al-Balushi of Penn State on in-situ stress measurements of thick N-polar InGaN films grown by MOCVD on C-Face SiC substrates.

Conclusion

In summary, the symposium featured more than 70 talks, as well as a poster session and a three-part tutorial, covering a wide variety of topics related to wide-bandgap materials targeted at solid-state lighting and power electronics applications. The symposium was well-attended and went very smoothly. The funds provided by ARO were critical in terms of providing financial support to both the tutorial speakers and the invited speakers, who served as the foundation of the successful technical program. ARO's support is gratefully acknowledged by the symposium organizers; the symposium would not have run as smoothly or been as successful without this support.

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Changes of electronic properties of AlGaIn/GaN HEMTs by surface treatment

W. Pletschen and St. Linkohr and L. Kirste and V. Cimalla and S. Müller and M. Himmerlich and S. Krischok and O. Ambacher

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t02-03](#)

doi: 10.1557/opl.2014.937, Published online by Cambridge University Press 18 Dec 2014

Growths of AlInN Single Layers and Distributed Bragg Reflectors for VCSELs

Y. Kozuka and K. Ikeyama and T. Yasuda and T. Takeuchi and S. Kamiyama and M. Iwaya and I. Akasaki

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t13-08](#)

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Stress engineering using AlN/GaN superlattices for epitaxy of GaN on 200 mm Si wafers

Jie Su and Eric A. Armour and Balakrishnan Krishnan and Soo Min Lee and George D. Papasouliotis

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t01-08](#)

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Wrap around field plate technique for GaN Schottky barrier diodes

Sowmya Kolli and Robert Hickman and Bruce W Alphenaar

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t02-07](#)

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Spatially resolved optical emission of cubic GaN/AlN multi-quantum well structures

D.J. As and R. Kemper and C. Mietze and T. Wecker and J.K.N. Lindner and P. Veit and A. Dempewolf and F. Bertram and J. Christen

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t03-03](#)

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Growth and Characterization of a-plane $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ / GaN hetrostructures on r-Sapphire

Shruti Mukundan and Lokesh Mohan and Greeshma Chandan and Basanta Roul and S.B.Krupanidhi

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Optimization of Carrier Distributions in Periodic Gain Structures toward Blue VCSELs

Kenjo Matsui and Kosuke Horikawa and Yugo Kozuka and Kazuki Ikeyama and Daisuke Komori and Tetsuya Takeuchi and Satoshi Kamiyama and Motoaki Iwaya and Isamu Akasaki

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t04-08](#)

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GaN HEMT Drain-Lag Performance Dependence on GaN Channel Quality

Yoichi Kamada and Naoya Okamoto and Masaru Sato and Atsushi Yamada and Junji Kotani and Tetsuro Ishiguro and Toshihiro Ohki and Shirou Ozaki and Kozo Makiyama and Keiji Watanabe and Kazukiyo Joshin

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Evaluation of electron overflow in nitride-based LEDs influenced by polarization charges at electron blocking layers

K. Hayashi and T. Yasuda and S. Katsuno and T. Takeuchi and S. Kamiyama and M. Iwaya and I. Akasaki

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Impact of Nitridation on Structural and Optical Properties of Epitaxial GaN Films Grown on M-Plane Sapphire by PAMBE

Shruti Mukundan and Lokesh Mohan and Greeshma Chandan and Basanta Roul and S.B. Krupanidhi

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MOCVD of GaN-based HEMT structures on 8 inch silicon substrates

Oleg Laboutin and Chien-Fong Lo and Chen-Kai Kao and Kevin O'Connor and Wayne Johnson and Daily Hill

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doi: 10.1557/opl.2015.100, Published online by Cambridge University Press 11 Feb 2015



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GaN/SiC Epitaxial Growth for High Power and High Switching Speed Device Applications

Zheng Sun and Shigeyoshi Usami and Di Lu and Takahiro Ishii and Marc Olsson and Kouhei Yamashita and Tadashi Mitsunari and Yoshio Honda and Hiroshi Amano

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t05-12](#)

doi: 10.1557/opl.2015.102, Published online by Cambridge University Press 11 Feb 2015

Fabrication and Lasing Properties of Single-Crystalline Semiconductor Microspheres with Anisotropic Crystal Structures

Shinya Okamoto and Satoshi Ichikawa and Yosuke Minowa and Masaaki Ashida

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t08-02](#)

doi: 10.1557/opl.2015.103, Published online by Cambridge University Press 11 Feb 2015

HVPE GaN with Low Concentration of Point Defects for Power Electronics

M. A. Reshchikov and J.D. McNamara and A. Usikov and H. Helava and Yu. Makarov

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t05-05](#)

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Low Resistive and Low Absorptive Nitride-Based Tunnel junctions

Daichi Minamikawa and Daiki Takasuka and Masataka Ino and Motoaki Iwaya and Tetsuya Takeuchi and Satoshi Kamiyama and Isamu Akasaki

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t03-04](#)

doi: 10.1557/opl.2015.139, Published online by Cambridge University Press 13 Feb 2015

GaN growth on silicon based substrates using pulsed electron beam deposition (PED) process

Nazmul Arefin and Matthew H. Kane and Preston R. Larson and Vince R. Whiteside and Khalid Hossain and Brittany N. Pritchett and Matthew B. Johnson and Patrick J. McCann

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t13-02](#)

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Pt/n-GaN metal-semiconductor and Pt/HfO₂/n-GaN metal-insulator-semiconductor Schottky diodes

Arjun Shetty and Basanta Roul and Shruti Mukundan and Greeshma Chandan and Lokesh Mohan and K J Vinoy and S B Krupanidhi

[MRS Online Proceedings Library, Volume 1736, 2015, mrsf14-1736-t02-08](#)

doi: 10.1557/opl.2014.938, Published online by Cambridge University Press 18 Dec 2014



Final Report for ARO Grant to Symposium NN, Mathematical and Computational Aspects of Materials Science

Organizers: Carme Calderer, Robert Lipton, Dionisios Margetis and Felix Otto

Materials science consistently delivers game changing advances in the way we live and the disciplines of applied and computational mathematics are increasingly central to these developments. Motivated by this exciting synergy the Symposium on Mathematical and Computational Aspects of Materials Science was held at last year's Materials Research Society Fall 2014 Meeting in Boston Massachusetts. The symposium brought together investigators working at the interface between materials science, mathematics and computational science. This symposium featured 16 invited lectures, 64 contributed talks and 40 posters. The organizing committee for this symposium is Carme Calderer, Robert Lipton, Dionisios Margetis, and Felix Otto.

The scientific and societal goals of this symposium were:

1. To foster new scientific collaborations between applied mathematicians and materials scientists in order to address contemporary problems at the frontiers of materials science.
2. Increase diversity and breadth of participation in STEM fields by exposing graduate students and early career applied mathematicians to contemporary and fundamental theoretical problems challenging materials science; enabling future breakthroughs through interdisciplinary collaboration.
3. To expose investigators with expertise in materials science disciplines to the latest applied mathematical and computational frameworks useful for the solution of challenging problems in materials science.

The financial support under this grant helped to defray travel expenses for 8 postdoctoral and pre-tenure faculty speakers participating in the Symposium on Mathematical and Computational Aspects of Materials Science at last year's Materials Research Society Fall 2014 Meeting. This meeting was held in Boston Massachusetts at the Hynes Convention Center from November 30 through December 5, 2014. The Symposium will run from December 1 through December 4, 2014.

The 8 junior speakers that received \$500 travel support under this grant were: Laurent Beland: Postdoc, Oak Ridge National Laboratory, Brian Wells: Graduate Student University of Massachusetts, Lowell, Daniel Hannah: Graduate Student Northwestern University, Christopher Hobbs: Undergraduate Student University of Tennessee, Knoxville, David Strubbe: Postdoc MIT, Changho Kim: Graduate Student, Brown University, Kamyar Davoudi: Graduate Student, Harvard University, and Paula Dassbach: Graduate Student, University of Minnesota, Minneapolis.

The proceedings of the symposium are published in Volume 1753 - 2014 MRS Fall Meeting - Symposium NN in the MRS Online Proceedings Library Hosted by Cambridge University Press, Cambridge Journals Online.

The topics covered in this symposium included:

- Biomaterials
- Phase transitions

- Massively parallel tools for computation for optical properties
- Metamaterials engineering
- Dynamics of liquid crystals
- New computational methods for materials discovery
- Density functional theory and semi-classical approximations

The research content of the 140 papers presented in this symposium has direct bearing on the basic research portfolios of the Army Research Office in the both the physical and engineering sciences. The papers presented in this symposium lie at the interface of materials science and the mathematical and computational sciences. The talks and posters presented in this symposium addressed topics in condensed matter physics, atomic and molecular physics, relationships between macromolecular architecture and material properties, microphysiology, systems biology, tissue engineering, applications and design of metamaterials, dynamics of systems far from equilibrium, and new computational and mathematical methods for materials discovery.

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Diffusion Wavelet Decomposition for Coarse-Graining of Polymer Chains
B. Christopher Rinderspacher and Jaydeep P. Bardhan and Ahmed E. Ismail

[MRS Online Proceedings Library, Volume 1753, 2015, mrsf14-1753-nn01-09](#)

doi: 10.1557/opl.2015.106, Published online by Cambridge University Press 11 Feb 2015

Recent Developments in Material Microstructure: a Theory of Coarsening
K. Barmak and E. Eggeling and M. Emelianenko and Y. Epshteyn and D. Kinderlehrer and R. Sharp and S. Ta'asan

[MRS Online Proceedings Library, Volume 1753, 2015, mrsf14-1753-nn01-01](#)

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Role of hydration forces in the properties of electrolyte solutions in the bulk and at interfaces
Maria L. Sushko and Kevin M. Rosso

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Parallelization of Molecular-Dynamics Simulations Using Tasks
Ralf Meyer and Chris M. Mangiardi

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2d And 3d Acoustic Metamaterials Using Space Coil Design
Santosh K. Maurya and Manu Sahay and Shobha Shukla and Sumit Saxena

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A Poroelastic-Viscoelastic Limit for Modeling Brain Biomechanics
Md. Mehedi Hasan and Corina S. Drapaca

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doi: 10.1557/opl.2015.111, Published online by Cambridge University Press 12 Feb 2015

Optimization-Based Coupling of Nonlocal and Local Diffusion Models
Marta D'Elia and Pavel B. Bochev

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Validity of the Free Electron Model for Two-Dimensional Electrodes
Kenji Kondo

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doi: 10.1557/opl.2015.112, Published online by Cambridge University Press 12 Feb 2015

The Vacancy Effect on Thermal Interface Resistance between Aluminum and Silicon by Molecular Dynamics
Yingying Zhang and Xin Qian and Zhan Peng and Nuo Yang

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Application of Bogoliubov-de Gennes equations to vortices in Hubbard superconductors
Chumin Wang and César G. Galván and Luis A. Pérez

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Numerics for Liquid Crystals with Variable Degree of Orientation
Ricardo H. Nochetto and Shawn W. Walker and Wujun Zhang

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Determining Upconversion Parameters and Invertibility of Nonlinear Dynamical Systems
Makhin Thitsa and Thanh Q. Ta

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Interface Stability Analysis of a Gel Material Surrounded by Air
Carlos A. Garavito Garzon and M. Carme. Calderer and Satish Kumar

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Scaffold Architecture and Properties for Osteoblasts Cell Culture: An Optimization Model and Application by Genetic Algorithm
Maraolina Domínguez-Díaz and Marco Antonio Cruz-Chavez

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Building a Coarse-Grained Model Based on the Mori-Zwanzig Formalism
Hee Sun Lee and Surl-Hee Ahn and Eric F. Darve

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Length Matters: Keeping Atomic Wires in Check
Brian Cunningham and Tchavdar N. Todorov and Daniel Dundas

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Mathematical Modeling of Thermomechanical Stresses of Multilayer Erosion-Resistant Electrode Coatings of Magnetically Controlled MEMS
Sergey Karabanov and Dmitry Suvorov and Gennady Gololobov and Evgeny Slivkin and Dmitry Tarabrin

[MRS Online Proceedings Library, Volume 1753, 2015, mrsf14-1753-nn03-01](#)

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Lithium-ion Diffusion in Solid Electrolyte Interface (SEI) Predicted by Phase Field Model
Pengjian Guan and Lin Liu

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